3-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-1-ol
6318-30-5 | DTXSID40282782

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.88e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 7.80e-01

Nearest Neighbors from the Training Set

Image not found
2-(2-Butoxyethoxy)ethanol
Measured: 7.44e-11
Predicted: 5.15e-11

Image not found
1-Butoxy-2-propanol
Measured: 3.76e-11
Predicted: 3.73e-11

Image not found
Butane, 1,1'-[methylenebis(oxy)]bis-
Measured: 3.39e-11
Predicted: 3.22e-11

Image not found
1,8-Cineol
Measured: 1.11e-11
Predicted: 1.72e-11